



# LIANG WANG

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## Education

### National University of Singapore

*Visiting Ph.D. Student*

Singapore

2025 - 2026 (expected)

- Lab: [ZhangLab/DeepMed](#), focusing on AI for Science
- Advisor: Prof. [Yang Zhang](#)    Mentor: Dr. [Zhiyuan Liu](#)
- Research Interests: Multi-modal Molecular Generation, Diffusion Models, Multi-modal LLMs

### Institution of Automation, Chinese Academy of Sciences

*Ph.D. in Pattern Recognition and Intelligent Systems (selected for the PhD honors program)*

Beijing, China

2021 - 2026 (expected)

- Lab: Center for Research on Intelligent Perception and Computing ([CRIPAC](#)), State Key Laboratory of Multimodal Artificial Intelligence Systems ([MAIS](#))
- Advisor: Prof. [Liang Wang](#)    Co-advisors: Prof. [Shu Wu](#) and Prof. [Qiang Liu](#)
- Research Interests: AI for Science, Graph Machine Learning, Data Mining

### Tongji University

*B.Eng. in Software Engineering*

Shanghai, China

2017 - 2021

- GPA: 4.86/5.00 (Ranking 3/214, Top 1.4%)
- Honors and Awards: National Scholarship (Top 1%), Outstanding Graduate of Shanghai (Top 5%)

## Selected Publications

### MolSpectra: Pre-training 3D Molecular Representation with Multi-modal Energy Spectra

- [Liang Wang](#), Shaozhen Liu, Yu Rong, Deli Zhao, Qiang Liu, Shu Wu, Liang Wang
- *ICLR 2025*

### Pin-Tuning: Parameter-Efficient In-Context Tuning for Few-Shot Molecular Property Prediction

- [Liang Wang](#), Qiang Liu, Shaozhen Liu, Xin Sun, Shu Wu, Liang Wang
- *NeurIPS 2024*

### Rethinking Graph Masked Autoencoders through Alignment and Uniformity

- [Liang Wang](#)<sup>\*</sup>, Xiang Tao<sup>\*</sup>, Qiang Liu, Shu Wu, Liang Wang
- *AAAI 2024*

### DIVE: Subgraph Disagreement for Graph Out-of-Distribution Generalization

- Xin Sun, [Liang Wang](#), Qiang Liu, Shu Wu, Zilei Wang, Liang Wang
- *KDD 2024*

### GSLB: The Graph Structure Learning Benchmark

- Zhixun Li, [Liang Wang](#), Xin Sun, Yifan Luo, Yanqiao Zhu, Dingshuo Chen, Yingtao Luo, Xiangxin Zhou, Qiang Liu, Shu Wu, Liang Wang, Jeffrey Xu Yu
- *NeurIPS 2023*

### Bi-Level Graph Structure Learning for Next POI Recommendation

- [Liang Wang](#), Shu Wu, Qiang Liu, Yanqiao Zhu, Xiang Tao, Mengdi Zhang, Liang Wang
- *IEEE Transactions on Knowledge and Data Engineering 2024*

### Semantic Evolvment Enhanced Graph Autoencoder for Rumor Detection

- Xiang Tao, [Liang Wang](#), Qiang Liu, Shu Wu, Liang Wang
- *WWW 2024*

### Chain-of-History Reasoning for Temporal Knowledge Graph Forecasting

- Yuwei Xia, Ding Wang, Qiang Liu, [Liang Wang](#), Shu Wu, Xiaoyu Zhang
- *ACL 2024 (Findings)*

## Selected Projects

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### PyGCL: A PyTorch Library for Graph Contrastive Learning

<https://github.com/PyGCL/PyGCL>

- ☆ Github Star: 919
- An easy-to-use library for graph contrastive learning with PyTorch. It implements a wide variety of contrastive objectives, data augmentations, contrasting modes and other utilities useful for implementing and evaluating contrastive learning on graphs.

### GSLB: A Benchmark of Graph Structure Learning

<https://github.com/GSL-Benchmark/GSLB>

- ☆ Github Star: 112
- An open-source library built for easy implementation and evaluation of graph structure learning model family. It offers a versatile control of graph dataset loading, structure learners, structure processors, and a bunch of reproduced models.

## Internship

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### AI4Science Group, Alibaba DAMO Academy

Hangzhou, China

*Research Intern*

*Aug. 2024 - Mar. 2025*

- Advised by Dr. [Yu Rong](#) and Dr. [Tingyang Xu](#).
- Conducted research on AI for chemistry and life science. The research work has been published in ICLR 2025.

### Graph Learning Group, NLP Center, Meituan Inc.

Beijing, China

*Research Intern*

*Sept. 2021 - Oct. 2022*

- Conducted research on graph self-supervised learning and graph-based spatial-temporal data mining. The research works have been published in IEEE TKDE and SDM 2024.

### Advertising Department, ByteDance Inc.

Shanghai, China

*Machine Learning Engineer Intern*

*Jul. 2020 - Dec. 2020*

- Supported the improvement of advertising machine learning models, and the development of the advertising system.

## Talks

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**Molecular Spectroscopy**, at Alibaba DAMO Academy, 2024, [Slides](#)

**Molecular Representation Learning and Property Prediction**, Invited by DP Technology, 2024, [Slides](#)

**Denoising-based 3D Molecular Pre-training**, 2024, [Slides](#)

**Generative Graph Self-Supervised Learning**, 2023, [Slides](#)

**Graph Transformers**, 2022, [Slides](#)

**Graph Self-Supervised Learning and Pre-Training**, 2021, [Slides](#)

## Academic Services

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**Conference Reviewers:** NeurIPS 2024 2025, ICLR 2025, ICML 2025, KDD 2024 2025, AISTATS 2025

**Journal Reviewers:** IEEE TKDE

## Technical Skills

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**Programming Languages:** Python, C++, Matlab, Java, C#

**Machine Learning Frameworks:** PyTorch, PyTorch Geometric (PyG), Deep Graph Library (DGL)

**Others:**  $\text{\LaTeX}$ , Git